# Electronic States in Diffused Quantum Wells

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## Abstract

In the present study we calculate the energy values and the spatial distributions of the bound electronic states in some diffused quantum wells. The calculations are performed within the virtual crystal approximation, $sp^3s^*$ spin dependent empirical tight-binding model and the surface Green function matching method. A good agreement is found between our results and experimental data obtained for $AlGaAs/GaAs$ quantum wells with thermally induced changes in the profile at the interfaces. Our calculations show that for diffusion lengths $L_D$=20 ÷ 100 Å the transition $(C3 - HH3)$ is not sensitive to the diffusion length, but the transitions $(C1 - HH1)$, $(C1 - LH1)$, $(C2 - HH2)$ and $(C2 - LH2)$ display large "blue shifts" as $L_D$ increases. For diffusion lengths $L_D$=0 ÷ 20 Å the transitions $(C1 - HH1)$ and $(C1 - LH1)$ are less sensitive to the $L_D$ changes than the $(C3 - HH3)$ transition. The observed dependence is explained in terms of the bound states spatial distributions.

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# I. INTRODUCTION

The $Al_xGa_{1-x}As/GaAs$ heterostructures have non-abrupt interfaces due to unwanted diffusion of $Al$ and $Ga$ across the heterojunctions. These compositionally graded interfaces change the electronic and optical properties of the quantum well structures [1-11]. A detailed study about the diffusion influence on the quantum well electronic states allows to control and use the new features these systems display. A comparison between calculated and measured transition energies permits to find diffusion coefficients for different temperatures [2,4,7,8]. Till now quantum wells with compositional grading at the interfaces were studied mainly using effective mass models and the envelope function approximation [1-4,6,8,9,11]. We believe that realistic tight-binding calculations will give a new information for these systems as was illustrated in [5] for an $AlAs/GaAs$ quantum well with a linear concentration profile at the interfaces.

In the present paper we study the influence of the diffusion length $L_D$ on the optical transitions energies in an interdiffused $Al_{0.2}Ga_{0.8}As/GaAs$ quantum well with an as-grown well width of 100 Å. This well was fabricated and experimentally studied in Ref.[1]. The energies of the transitions $(C1 - HH1)$, $(C1 - LH1)$ and $(C2 - HH2)$ were measured at temperature 2 K for $L_D$=0, 18, 20, 28, 48.5 and 66 Å after annealing at 950 C for different time durations.

# II. MODEL AND METHOD

The data of the system under study are taken from Ref.[1]. The width of the initial (as-grown) $Al_{0.2}Ga_{0.8}As/GaAs$ rectangular quantum well is 100 Å. The $Al$ composition across the well after the diffusion can be found from the expression: (See fig.1.)

$$C(z) = C_b + (C_w - C_b)/2 \left[ \mathtt{erf}\,(h - z)/L_D + \mathtt{erf}\,(h + z)/L_D \right], \tag{1}$$

where $C(z)$ is the $Al$ concentration at a distance $z$ from the well center; $C_w$, the $Al$ concentration in the well before the diffusion; $C_b$, the $Al$ concentration in the barrier before the diffusion; $2h$, the width of the initial well; $L_D$, the diffusion length. The Eq.(1) is widely used in the literature (see for instance Ref.[1]).

We use the $sp^3s^*$ spin dependent empirical tight binding model, the virtual crystal approximation and the surface Green function matching technique [12-15]. For more details see [12] and references therein. The calculations were performed at the center of the two-dimensional Brillouin zone for the (100) growth direction.

Each diffused structure was divided into three regions, namely, the external homogeneous barriers with negligible diffusion (the $Al$ concentration in the planes of matching was 0.199) and the internal inhomogeneous (diffused) well region having a concentration profile as determined from Eq.(1). The size of the inhomogeneous slab was 167, 131, and 95 monolayers respectively for $L_D$=100, 70 and 35 Å. The Green function of the external barriers was calculated from the transfer matrix in the usual way and the Green function of the diffused well region, by means of the algorithm established and used to study other heterogeneous structures [12,13,15].

## III. RESULTS AND DISCUSSION

We calculated the energies of the first three bound electron states $C1$, $C2$, $C3$ (see fig.2a) and the first five hole states $HH1$, $LH1$, $HH2$, $HH3$ and $LH2$ (see fig.2b) in the studied quantum well for different diffusion lengths $L_D$. The calculations in the interval $L_D = 0 \div 70$ Å were performed through 5 Å and in the interval $L_D = 70 \div 100$ Å - through 10 Å. We also found the bound states energies for the diffusion lengts $L_D$=0, 18, 20, 28, 48.5 and 66 Å. (The measurements in [1] were conducted with these diffusion lengths values.) As $L_D$ increases the bound states depart further from the $GaAs$ band edges. Qualitatively similar results have been reported in [5] for an $AlAs/GaAs$ quantum well with linearly graded interfaces. As a difference from [5], in our case the energies of the states $C3, HH3$ and $LH2$ change several times less than the energies of the states $C1, C2, HH1, HH2$ and $LH1$. For instance, over the whole interval $L_D = 0 \div 70$ Å the state $C3$ rises only by 8 meV while over the same interval the state $C1$ rises by 61 meV. The states $HH3$ and $HH1$ change by 19 meV and 36 meV respectively over the same diffusion length interval.

To understand the above mentioned behaviour we calculated the spatial distributions of all bound states for all diffusion lengths. The diffusion modifies the initial (as-grown) quantum well and leads to formation of two regions in the diffused well. In the as-grown well region (see fig.1) the $Al$ concentration increases and the energies of the bound electron (hole) states in the diffused quantum well increase (decrease). (The energy zero is at the $AlAs$ valence band top edge.) On the contrary, in the as-grown barrier region (see fig.1) the $Al$ concentration decreases and the energies of the bound states decrease (increase) for electrons (holes). All bound states are more concentrated in the as-grown well region and consequently their energies increase (decrease) for electrons (holes) as $L_D$ increases. But, in general, a competition exists between two regions affected by the diffusion and a compensation of the energy shifts can occur. The magnitude of the energy shift for a given bound state depends on the relation between the probabilities of this state to occupy the diffused well part with increased $Al$ concentration (the as-grown well region) and with decreased $Al$ concentration (the as-grown barrier region). As an example, in order to illustrate the role of the above mentioned compensation, the spatial distributions of the electron states $C3$ and $C1$ are shown in fig.3a and fig.3b for the as-grown and a diffused ($L_D$=35Å) quantum well. The energy of the state $C3$ changes only by 7 meV because this state spreads over both regions affected by the diffusion (within and outside the initial well, see fig.3a) and the compensation occurs. The hole state $HH3$ has a similar spatial distribution and also shifts weakly. The energy of the state $C1$ shifts with 21 meV due to its spatial localization in the central well region with increased $Al$ concentration after the diffusion (see fig.3b) and the compensation does not occur. The same argument is valid for the hole states $HH1$ and $LH1$.

Theoretical curves of the transition energies dependence on the diffusion length $L_D$ for the transitions $(C1 - HH1)$, $(C1 - LH1)$, $(C2 - HH2)$, $(C2 - LH2)$ and $(C3 - HH3)$ are shown in fig.4a for $Al_{0.2}Ga_{0.8}As/GaAs$ diffused quantum wells. There is a "blue shift" for all transitions with $L_D$ increasing as reported in [2,4] for similar systems. This shift is 27 meV for $(C3 - HH3)$ and 97 meV for $(C1 - HH1)$ as $L_D$ increases from 0 to 70 Å. The transitions $(C1 - LH1)$, $(C2 - HH2)$ and $(C2 - LH2)$ shift by 94 meV, 82 meV and 65 meV respectively.

The transition $(C3 - HH3)$ is not sensitive to the diffusion length for $L_D$=20 $\div$ 100 Å

because the energies of the states $C3$ and $HH3$ change weakly, see fig.2. A relatively low sensitivity of the transition $(C3 - HH3)$ to the diffusion length was measured in [2]. The transitions $(C1 - HH1)$, $(C1 - LH1)$ and $(C2 - HH2)$ show considerable "blue shifts" in the interval $L_D$=20÷100 Å because the energies of the states $C1$, $C2$, $HH1$, $LH1$ and $HH2$ change significantly, see fig.2.

For low diffusion length values ($L_D \leq 20$ Å) the transition $(C3 - HH3)$ is sensitive to the $L_D$ changes because the energies of the states $C3$ and $HH3$ depend strongly on the diffusion length, see fig.2. The $Al$ concentration changes only near the interfaces and the spatial distributions of the states $C3$ and $HH3$ do not allow a compensation. In this diffusion length interval the transitions $(C1 - HH1)$ and $(C1 - LH1)$ are less sensitive to the $L_D$ changes due to the energies of the states $C1$, $HH1$ and $LH1$ depend on $L_D$ weaker than the $C3$ and $HH3$ energies, see fig.2. The states $C1$, $HH1$ and $LH1$ are mainly localized in the central well part where the $Al$ concentration is not affected.

In fig.4b we compare our theoretical curves with the experimental curves from [1] for $(C1 - HH1)$, $(C1 - LH1)$ and $(C2 - HH2)$ transitions energies with $L_D$=0, 18, 20, 28, 48.5 and 66 Å. The measurements in [1] have been conducted at temperature 2 K and temperature corrections of the theoretical values were not necessary. It is obvious that the agreement with the experimental data is quite satisfactory inspite of the fact that excitonic effects were not taken into account and fit was not done. All experimental curves lie about 10 ÷ 45 meV below the theoretical ones. The agreement between the theory and the experiment is better for the excited states than the ground states due to the fact that the exciton binding energies are higher for the ground states. For all transitions in fig.4b two curves (a theoretical and the experimental) diverge with $L_D$ increasing. For instance, for $L_D$=0 Å the discrepances are 29 meV, 30 meV and 10 meV for the transitions $(C1 - HH1)$, $(C1 - LH1)$ and $(C2 - HH2)$, respectively, and for $L_D$=66 Å 45 meV, 41 meV and 29 meV respectively. A possible explanation of this behaviour could be an increase of the excitonic binding energy for higher $L_D$ values due to the higher $Al$ concentration within the initial well region. This means that the excitons are localized even in the case of $L_D$=66 Å. The spatial distributions of the bound states for these diffusion lengths support such an assumption. An exciton binding energy increase has been reported in [4] for double-barrier quantum wells as $L_D$ increases.

## IV. CONCLUSION

In the present paper we performed numerical calculations which showed that the empirical tight-binding model combined with the surface Green function matching method and the algorithm for treating inhomogeneous finite slabs [12-15] works very well in case of quantum wells with graded interfaces. We found that the theoretical dependence of the transition energies on the diffusion lengths is in good agreement with the experiment.

For given as-grown well width and diffusion length $L_D$, the sensitivity of the transitions to $L_D$ changes depends on the bound states spatial distributions over the diffused well regions. For small $L_D$ values (in our case below 20 Å) the transition $(C3 - HH3)$ is more sensitive to the $L_D$ changes than the transitions $(C1 - HH1)$ and $(C1 - LH1)$. For large $L_D$ values (in our case above 20 Å) the transition $(C3 - HH3)$ is not sensitive to the diffusion length, but the transitions $(C1 - HH1)$ and $(C1 - LH1)$ display large "blue shifts".

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## ACKNOWLEDGMENTS

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## FIGURES

FIG. 1. Al concentration profiles of quantum wells for diffusion lengths $L_D$=0, 25, 50 and 100 Å. The value of $L_D$=0 Å corresponds to the initial as-grown rectangular quantum well of 100 Å (35 monolayers).

FIG. 2. (a) Electron energy levels (in eV) of the states $C1$, $C2$ and $C3$, (b) hole energy levels (in eV) of the states $HH1$, $LH1$, $HH2$, $HH3$ and $LH2$ for diffused quantum wells, as a function of the diffusion length $L_D$ (in Å). The value of $L_D$=0 Å corresponds to the well width of 100 Å (35 monolayers) of the initial as-grown rectangular quantum well. The energy zero is at the $AlAs$ valence band top edge.

FIG. 3. Spatial distributions of $C3$ (a) and $C1$ (b) electron bound states over the as-grown (solid lines) and diffused (dotted lines) quantum wells. The diffusion length is $L_D$=35 Å. The bound states energies are: $C3$ (as-grown well) - 2.240 eV, $C3$ (diffused well) - 2.247 eV; $C1$ (as-grown well) - 2.118 eV, $C1$ (diffused well) - 2.139 eV.

FIG. 4. Transition energies (in eV) for diffused quantum wells, as a function of the diffusion length $L_D$ (in Å). The value of $L_D$=0 Å corresponds to the well width of 100 Å (35 monolayers) of the initial as-grown rectangular quantum well. (a) theory; transitions $(C1 - HH1)$, $(C1 - LH1)$, $(C2 - HH2)$, $(C2 - LH2)$ and $(C3 - HH3)$. (b) theory (th.) and experiment (exp.); transitions $(C1 - HH1)$, $(C1 - LH1)$ and $(C2 - HH2)$.